Numerical solutions of partial differential equations

Frames 1 to 64

Learning outcomes

When you have completed this Programme you will be able to:

- Derive the finite difference formulas for the first partial derivatives of a function of two real variables and construct the central finite difference formula to represent a first-order partial differential equation
- Draw a rectangular grid of points overlaid on the domain of a function of two real variables and evaluate the function at the boundary grid points
- Construct the computational molecule for a first-order partial differential equation in two real variables and use the molecule to evaluate the solutions to the equation at the grid points interior to the boundary
- Describe the solution as a set of simultaneous linear equations and use matrices to represent them
- Invert the coefficient matrix and thereby represent the solution to the partial differential equation as a column matrix
- Take account of a boundary condition in the form of the derivative normal to the boundary
- Obtain the central finite difference formulas for the second derivatives of a function of two real variables and construct finite difference formulas for second-order partial differential equations
- Use the forward difference formula for the first time derivatives in partial differential equations involving time and distance
- Use the Crank–Nicolson procedure for a partial differential equation involving a first time derivative
- Appreciate the use of dimensional analysis in the conversion of a partial differential equation modelling a physical system into a dimensionless equation

Introduction

1 The numerical solution of partial differential equations is a large subject and can form the content of a course in itself. Here we shall just introduce the subject by considering the basic methods of solving some first- and second-order partial differential equations that involve functions of two real variables. The approach that is used is to construct finite difference formulas for the first and second partial derivatives and then to construct a finite difference formula that represents an approximation to the differential equation. However, before we move into the realm of functions of two real variables we shall derive the finite difference formulas for the ordinary first derivative of a function of a single real variable.

Next frame

Numerical approximation to derivatives

2 A function of one real variable $f(x)$ has the Taylor series expansion

$$f(x+h)=f(x)+hf'(x)+\frac{h^2}{2!}f''(x)+\frac{h^3}{3!}f'''(x)+\dots$$

and, equally, replacing h by $-h$

$$f(x-h)=f(x)-hf'(x)+\frac{h^2}{2!}f''(x)-\frac{h^3}{3!}f'''(x)+\dots$$

From the first equation we can see that by dividing through by h, we have

$$\frac{f(x+h)-f(x)}{h}=f'(x)+\frac{h}{2!}f''(x)+\frac{h^2}{3!}f'''(x)+\dots$$

and from the second equation

$$\frac{f(x-h)-f(x)}{h}=-f'(x)+\frac{h}{2!}f''(x)-\frac{h^2}{3!}f'''(x)+\dots$$

If we now neglect terms of the order two and higher we see that

$$f'(x)\approx\frac{f(x+h)-f(x)}{h}$$ [this is the *forward difference formula* for the first derivative of $f(x)$]

and

$$f'(x)\approx\frac{f(x)-f(x-h)}{h}$$ [this is the *backward difference formula* for the first derivative of $f(x)$]

and both of these are accurate up to terms of order two. A more accurate estimate of the derivative can be obtained by subtracting the two Taylor series expansions from each other to get

$f'(x) \approx$ .... neglecting terms of the order of ....

3

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

neglecting terms of the order two and higher

Because

$$\begin{aligned} f(x+h) - f(x-h) &= \left(f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots\right) \\ &\quad - \left(f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \dots\right) \\ &= 2\left(hf'(x) + \frac{h^3}{3!}f'''(x) + \dots\right) \end{aligned}$$

and so

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2}{3!}f'''(x) + \dots$$

giving

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

neglecting terms of the order two and higher.

The derivative at x is given as the difference between the two values either side of $f(x)$ divided by $2h$.

This is called the *central difference formula* for the derivative of $f(x)$ and because it is the most accurate of the three for small h, it is the one that we shall use in the remainder of the Programme.

Now we need to look at the second derivative. By adding the first two Taylor series expansions in Frame 2 we find that

$f''(x) \approx$ .... neglecting terms of the order ....

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$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$
neglecting terms of the order two and higher

Because

$$f(x+h) + f(x-h) = \left(f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \dots\right)$$
$$+ \left(f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \dots\right)$$
$$= 2\left(f(x) + \frac{h^2}{2!}f''(x) + \frac{h^4}{4!}f^{iv}(x) + \dots\right)$$
$$= 2f(x) + h^2 f''(x) + \frac{h^4}{12}f^{iv}(x) + \dots$$

and so

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{h^2}{12}f^{iv}(x) + \dots$$

Therefore

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$ neglecting terms of the order two and higher

This is the *central difference formula* for the second derivative and, as you see, it possesses the same level of accuracy as the central difference formula for the first derivative.

Functions of two real variables

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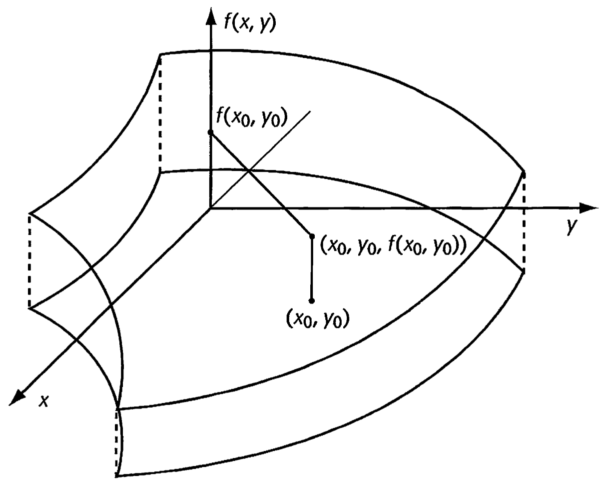
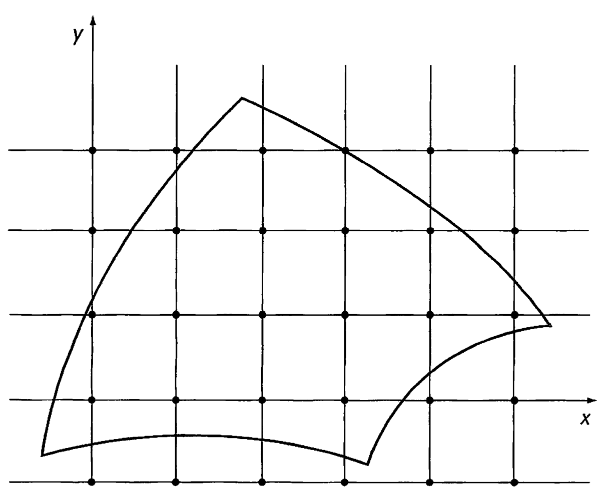
A function of two real variables $f(x, y)$ is graphically represented as a surface in three-dimensional space.



If $f(x, y)$ is single-valued, then to every *domain* point (x, y) there corresponds a single range point $f(x, y)$ and hence a single surface point $(x, y, f(x, y))$. If we know the exact form of $f(x, y)$ then we can compute its value at any domain point (x, y) selected at random. If we do not know the exact form of $f(x, y)$ but we do know that it satisfies a given differential equation then to evaluate $f(x, y)$ numerically we have to be more systematic. What we do is to lay a rectangular grid over the domain and evaluate $f(x, y)$ at the grid points – the points of intersection of the lines parallel with the x-axis and the lines parallel with the y-axis.



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In this Programme we shall be considering functions of two real variables that satisfy given differential equations and whose domains are restricted to being rectangular. This restriction avoids many of the problems that occur with arbitrary domain shapes where the grid lines can cross the domain boundary.

Grid values

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The rectangular domain of the function is overlaid by a grid whose mesh size is of h units in the x direction and k units in the y direction. We shall denote the value of $f(x, y)$ at the ijth grid point as

$$f_{i,j} \equiv f(ih, jk)$$

The values of the expression $f(x, y)$ are required to be found at the grid points as shown:

$$\begin{array}{ccccc}
\cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & f_{i-1,j+1} & f_{i,j+1} & f_{i+1,j+1} & \cdots \\
\cdots & f_{i-1,j} & f_{i,j} & f_{i+1,j} & \cdots \\
\cdots & f_{i-1,j-1} & f_{i,j-1} & f_{i+1,j-1} & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots
\end{array}$$

Notice as you move along the jth row of this table that the value of y is constant at $y_j = y_0 + jk$ for all points on that row. Similarly, as you move up and down the ith column that the value of x is constant at $x_i = x_0 + ih$ for all points in that column. These facts now enable us to define the central difference formulas for the partial derivatives of $f(x, y)$.

The first partial derivative of $f(x, y)$ with respect to the variable x is obtained by differentiating $f(x, y)$ with respect to x whilst keeping the value of the variable y constant. Therefore, as with the ordinary derivative

$\left.\dfrac{\partial f(x, y)}{\partial x}\right|_{ij}$ *is equal to the difference between the two adjacent values of $f(x, y)$ in the x-direction divided by twice the mesh size in the x-direction.*

That is

$$\left.\frac{\partial f(x, y)}{\partial x}\right|_{-ij} = \frac{f_{i+1,j} - f_{i-1,j}}{2h}$$

This is the central difference formula for the partial derivative with respect to x. Similarly, the central difference formula for the partial derivative with respect to y is

$$\left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = \ldots\ldots\ldots\ldots$$

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$$\boxed{\left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = \frac{f_{i,j+1} - f_{i,j-1}}{2k}}$$

Because

$\left.\dfrac{\partial f(x, y)}{\partial y}\right|_{ij}$ *is equal to the difference between the two adjacent values of $f(x, y)$ in the y-direction divided by twice the mesh size in the y-direction.*

That is

$$\left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = \frac{f_{i,j+1} - f_{i,j-1}}{2k}$$

Let's try an example so that we can put all this information together.

Example 1

Find the solution to $3\dfrac{\partial f(x, y)}{\partial x} - 4\dfrac{\partial f(x, y)}{\partial y} = 0$, for $0 \leq x \leq 1$ and $0 \leq y \leq 1$ given that the boundary conditions are

$$f(x, 0) = 4x + 4$$
$$f(x, 1) = 4x + 7$$
$$f(0, y) = 3y + 4$$
$$f(1, y) = 3y + 8$$

for a mesh of size 1/4 in the x-direction and of size 1/3 in the y-direction.

Next frame

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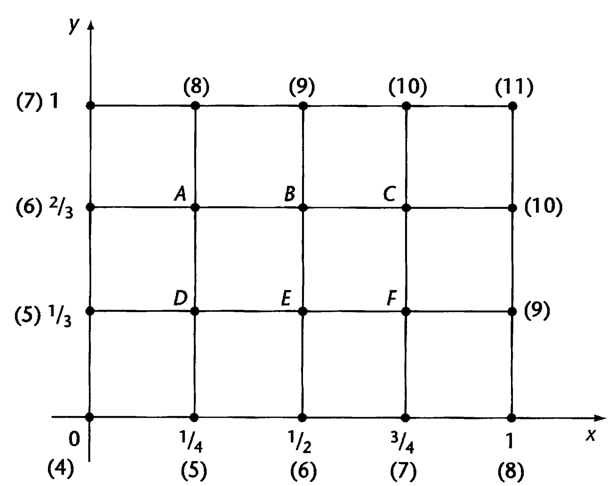
The first thing we must do is to make a reasonable drawing of the domain of the function with the grid overlaid. The domain of $f(x, y)$ is the square of side length 1 as shown in the diagram.



Overlaid on the function domain in the x–y plane is a mesh of grid points. The values of $f(x, y)$ that we can compute directly from the boundary conditions are shown in brackets. For example, from $f(x, 0) = 4x + 4$ we obtain $f(1/4, 0) = 5$, $f(1/2, 0) = 6$, $f(3/4, 0) = 7$ and $f(1, 0) = 8$. From $f(1, y) = 3y + 8$ we obtain $f(1, 0) = 8$, $f(1, 1/3) = 9$, $f(1, 2/3) = 10$ and $f(1, 1) = 11$. Notice that the value found at $f(1, 0) = 8$ using $f(x, 0) = 4x + 4$ is the same as the value found using $f(1, y) = 3y + 8$, as of course it must be. The values of $f(x, y)$ that we have to determine are labelled A to F.

The second part of the procedure is to find the central difference formula that describes the differential equation:

We have $\left.\dfrac{\partial f(x, y)}{\partial x}\right|_{ij} = \dfrac{f_{i+1,j} - f_{i-1,j}}{2h} = 2(f_{i+1,j} - f_{i-1,j})$ because $h = 1/4$

$\left.\dfrac{\partial f(x, y)}{\partial y}\right|_{ij} = \dfrac{f_{i,j+1} - f_{i,j-1}}{2k} = 1{\cdot}5(f_{i,j+1} - f_{i,j-1})$ because $k = 1/3$

Therefore

$$3\frac{\partial f(x, y)}{\partial x} - 4\frac{\partial f(x, y)}{\partial y} = 0 \text{ becomes } \dots\dots\dots\dots$$

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$$\boxed{6(f_{i+1,j} - f_{i-1,j}) - 6(f_{i,j+1} - f_{i,j-1}) = 0}$$

Because

$3\dfrac{\partial f(x, y)}{\partial x} - 4\dfrac{\partial f(x, y)}{\partial y} = 0$ evaluated at the ijth grid point is

$$3\left.\frac{\partial f(x, y)}{\partial x}\right|_{ij} - 4\left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = 0$$

which is

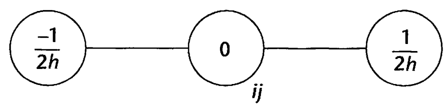
$$3 \times 2(f_{i+1,j} - f_{i-1,j}) - 4 \times 1{\cdot}5(f_{i,j+1} - f_{i,j-1}) = 0, \text{ that is}$$
$$6(f_{i+1,j} - f_{i-1,j}) - 6(f_{i,j+1} - f_{i,j-1}) = 0$$

Computational molecules

The value of the first derivative with respect to x at the point (x_i, y_j) on the grid overlaying the function domain is found by evaluating the right-hand side of the equation

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{ij} = \frac{f_{i+1,j} - f_{i-1,j}}{2h} = \frac{-f_{i-1,j} + f_{i+1,j}}{2h}$$

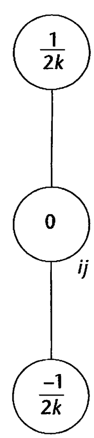
and this process is repeated for every grid point in the function domain. We can construct a graphic template to assist us in this process:



The three circles in a row are used to calculate the contribution of three adjacent row members to the equation. If the circle labelled *ij* is laid over the *ij*th grid point then the derivative at that point is given by multiplying the value of the function at the $i-1, j$ grid point (one to the left) by $-1/2h$ and adding the product of the value of the function at the $i+1, j$ grid point (one to the right) by $1/2h$. The number 0 in the centre circle means that we multiply $f_{i,j}$ by zero because it does not enter into the formula. This template is called a *computational molecule.* The horizontal structure reflects the fact that we are evaluating along a row. By a similar reasoning the first derivative with respect to y at the *ij*th grid point is

$$\left.\frac{\partial f(x,y)}{\partial y}\right|_{ij} = \frac{f_{i,j+1} - f_{i,j-1}}{2k}$$

and this is represented by the computational molecule:



The vertical structure reflects the fact that we are evaluating up and down a column.

By combining such computational molecules we can construct a composite molecule that represents the entire differential equation. For example, the partial differential equation

$$a\frac{\partial f(x, y)}{\partial x} + b\frac{\partial f(x, y)}{\partial y} = c$$

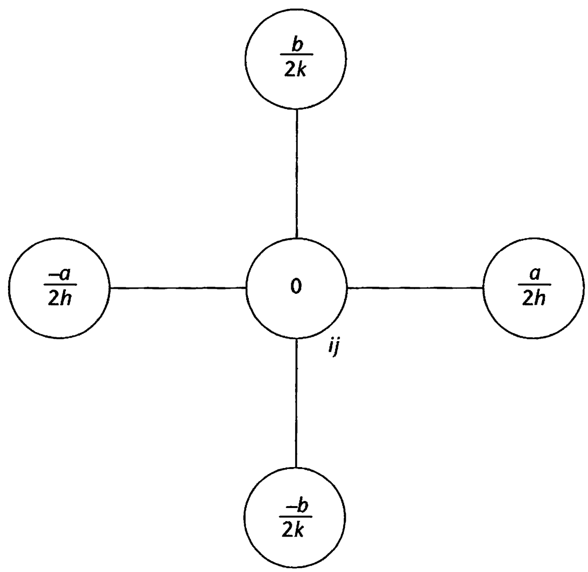
evaluated at the *ij*th grid point is

$$a\left.\frac{\partial f(x, y)}{\partial x}\right|_{ij} + b\left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = c$$

and is represented by the central difference formula

$$\frac{a}{2h}(f_{i+1,j} - f_{i-1,j}) + \frac{b}{2k}(f_{i,j+1} - f_{i,j-1}) = c$$

which is in turn represented by the composite computational molecule:



So the equation $3\frac{\partial f(x, y)}{\partial x} - 4\frac{\partial f(x, y)}{\partial y} = 0$ which is represented by the finite difference formula

$$6(f_{i+1,j} - f_{i-1,j}) - 6(f_{i,j+1} - f_{i,j-1}) = 0$$

has the computational molecule ....

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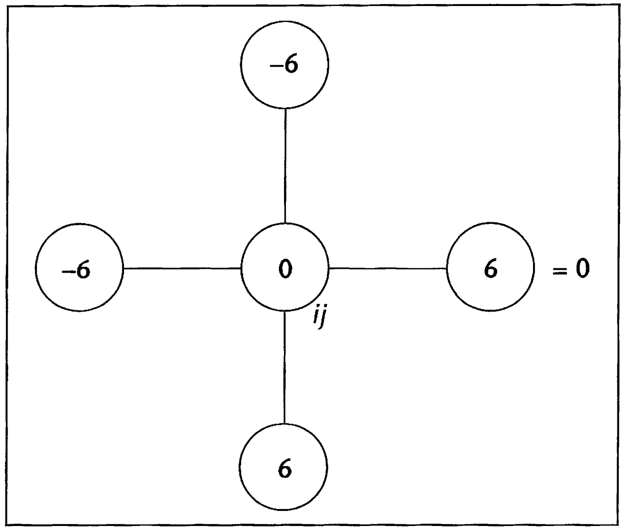

We now place the centre of the molecule, in turn, on each of the grid points at which we need to find the value of $f(x, y)$:

On A	$-36 - 48 + 6B + 6D = 0$
On B	$-6A - 54 + 6C + 6E = 0$
On C	....
On D	....
On E	....
On F	....

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On A	$-36 - 48 + 6B + 6D = 0$
On B	$-6A - 54 + 6C + 6E = 0$
On C	$-6B - 60 + 60 + 6F = 0$
On D	$-30 - 6A + 6E + 30 = 0$
On E	$-6D - 6B + 6F + 36 = 0$
On F	$-6E - 6C + 54 + 42 = 0$

We now have six simultaneous linear equations in six unknowns.

These can be written in matrix form as ....

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$$\begin{pmatrix} 0 & 6 & 0 & 6 & 0 & 0 \\ -6 & 0 & 6 & 0 & 6 & 0 \\ 0 & -6 & 0 & 0 & 0 & 6 \\ -6 & 0 & 0 & 0 & 6 & 0 \\ 0 & -6 & 0 & -6 & 0 & 6 \\ 0 & 0 & -6 & 0 & -6 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 84 \\ 54 \\ 0 \\ 0 \\ -36 \\ -96 \end{pmatrix}$$

That is: $\mathbf{Ax} = \mathbf{b}$ with solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$

There are many ways to derive the inverse matrix $\mathbf{A}^{-1}$, many of them time consuming and prone to arithmetic error. An efficient method in terms of time and accuracy is to use a spreadsheet, provided of course that the spreadsheet has the appropriate functionality. Here we shall use the *Microsoft Excel* spreadsheet which possesses matrix functions. If your spreadsheet does not have these functions then you are referred to Programme 12, Matrix algebra.

If you do possess the *Microsoft Excel* spreadsheet then follow the instructions in the next frame.

Next frame

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1 Open your spreadsheet.
2 Place the cell highlight in cell A1 and then enter the values of matrix **A** into the cells A1 to F6.
3 Place the cell highlight in cell H1 and then enter the values of matrix **b** into the cells H1 to H6.
4 Place the cell highlight in cell A8 and drag the mouse to highlight the block of cells A8 to F13 – this is where the inverse of **A** is going to go.
5 With this block of cells highlighted, type the function:

   =MINVERSE(A1:F6) and then press the three keys **Ctrl-Shift-Enter** together

   As you type, the function is entered into cell A8 and when you press the **Ctrl-Shift-Enter** keys together the block of cells A8 to F13 fills with entries. This block of cells is the inverse matrix $\mathbf{A}^{-1}$. (*Note*: You must remember to press the three keys **Ctrl-Shift-Enter** together. If you just press **Enter** it will not work.)

   MINVERSE(array) is the *Excel* function that computes the inverse of the square matrix denoted by **array**.

6 Place the cell highlight in cell H8 and drag the mouse to highlight the block of cells H8 to H13 – this is where the solution **x** is going to go.
7 With this block of cells highlighted type the function:

   =MMULT(A8:F13, H8:H13) and then press the three keys **Ctrl-Shift-Enter** together

   MMULT(array1,array2) is the *Excel* function that multiplies the two matrices denoted by **array1** and **array2**.

▶

As you type, the function is entered into cell H8 and when you press the **Ctrl-Shift-Enter** keys together the block of cells H8 to H13 fills with entries. This block of cells is the product matrix $\mathbf{A}^{-1}\mathbf{b}$, that is, the solution matrix $\mathbf{x}$.

$$\begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 7 \\ 8 \\ 9 \\ 6 \\ 7 \\ 8 \end{pmatrix}$$

These values are identical to the values found from the exact solution which is $f(x, y) = 4x + 3y + 4$.

Next frame

Summary of procedures

15 The procedure to solve a first-order partial differential equation requires a number of steps to be completed in a certain order, and the following list describes the sequence:

1 Draw the domain of the function with the grid overlaid.
2 On the drawing enter the values of $f(x, y)$ that can be obtained from the boundary conditions.

Put these values in brackets so that they will be easily distinguished from the x- and y-values on the axes.

3 Label the grid points at which $f(x, y)$ is to be evaluated with capital letters.
4 Construct the central difference equation that represents the numerical approximation to the partial differential equation.
5 Construct the computational molecule for this equation.
6 Lay the centre of the molecule on each of the lettered grid points in turn and derive a set of simultaneous linear equations – the unknowns being represented by the letters at the grid points.
7 Write the simultaneous linear equations in matrix form $\mathbf{Ax} = \mathbf{b}$.
8 Find the inverse matrix $\mathbf{A}^{-1}$ and compute the solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$.

Now try one yourself. Just follow the procedure in order and you should have no problems.

▶

Example 2

The solution to $x\dfrac{\partial f(x, y)}{\partial x} - y\dfrac{\partial f(x, y)}{\partial y} = 0$, for $0 \leq x \leq 1$ and $0 \leq y \leq 1$ given that

$f(x, 0) = 2$
$f(x, 1) = x + 2$
$f(0, y) = 2$
$f(1, y) = y + 2$

for a mesh of $1/4$ in the x-direction and $1/3$ in the y-direction is:

. . . .

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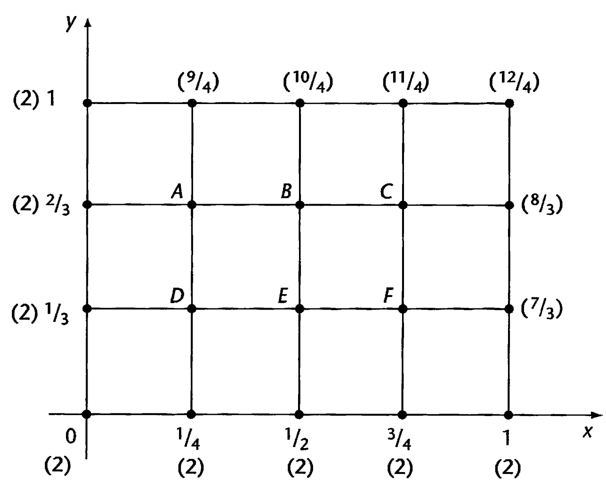
$$\begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 2{\cdot}166\ldots \\ 2{\cdot}33\ldots \\ 2{\cdot}5 \\ 2{\cdot}0833\ldots \\ 2{\cdot}166\ldots \\ 2{\cdot}25 \end{pmatrix} = \begin{pmatrix} 13/6 \\ 7/3 \\ 5/2 \\ 25/12 \\ 13/6 \\ 9/4 \end{pmatrix}$$

Because

The domain of the function $f(x, y)$ with the overlaid grid looks as follows:



where the numbers at the grid points in brackets are the values of $f(x, y)$ obtained by applying the boundary conditions and the letters $A \ldots F$ represent the values of $f(x, y)$ that we have yet to determine.

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The central difference formulas for the two first partial derivatives of $f(x, y)$ are

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{ij} = \frac{f_{i+1,j} - f_{i-1,j}}{2h} = 2(f_{i+1,j} - f_{i-1,j}) \text{ because } h = 1/4$$

$$\left.\frac{\partial f(x,y)}{\partial y}\right|_{ij} = \frac{f_{i,j+1} - f_{i,j-1}}{2k} = 1{\cdot}5(f_{i,j+1} - f_{i,j-1}) \text{ because } k = 1/3$$

Therefore

$$x\frac{\partial f(x,y)}{\partial x} - y\frac{\partial f(x,y)}{\partial y} = 0 \text{ becomes } \ldots\ldots\ldots\ldots$$

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$$\boxed{2(x_i f_{i+1,j} - x_i f_{i-1,j}) - 1{\cdot}5(y_j f_{i,j+1} - y_j f_{i,j-1}) = 0}$$

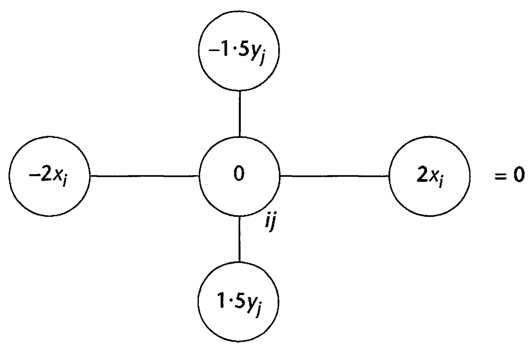
Because

$$x\frac{\partial f(x,y)}{\partial x} - y\frac{\partial f(x,y)}{\partial y} = 0$$

is written using the central difference formulas as

$$\begin{aligned} &2x_i(f_{i+1,j} - f_{i-1,j}) - 1{\cdot}5y_j(f_{i,j+1} - f_{i,j-1}) \\ &= 2(x_i f_{i+1,j} - x_i f_{i-1,j}) - 1{\cdot}5(y_j f_{i,j+1} - y_j f_{i,j-1}) = 0 \end{aligned}$$

This has the following computational molecule:



Placing the centre of the molecule, in turn, on each of the grid points that we need to evaluate, we obtain the six simultaneous equations:

On A at $(\frac{1}{4}, \frac{2}{3})$: $-2(\frac{1}{4})(2) - \frac{3}{2}(\frac{2}{3})(\frac{9}{4}) + 2(\frac{1}{4})B + \frac{3}{2}(\frac{2}{3})D = 0$

On B at $(\frac{1}{2}, \frac{2}{3})$: $-2(\frac{1}{2})A - \frac{3}{2}(\frac{2}{3})(\frac{10}{4}) + 2(\frac{1}{2})C + \frac{3}{2}(\frac{2}{3})E = 0$

On C at $(\frac{3}{4}, \frac{2}{3})$: $-2(\frac{3}{4})B - \frac{3}{2}(\frac{2}{3})(\frac{11}{4}) + 2(\frac{3}{4})(\frac{8}{3}) + \frac{3}{2}(\frac{2}{3})F = 0$

On D at $(\frac{1}{4}, \frac{1}{3})$: $-2(\frac{1}{4})(2) - \frac{3}{2}(\frac{1}{3})A + 2(\frac{1}{4})E + \frac{3}{2}(\frac{1}{3})(2) = 0$

On E at $(\frac{1}{2}, \frac{1}{3})$: $-2(\frac{1}{2})D - \frac{3}{2}(\frac{1}{3})B + 2(\frac{1}{2})F + \frac{3}{2}(\frac{1}{3})(2) = 0$

On F at $(\frac{3}{4}, \frac{1}{3})$: $-2(\frac{3}{4})E - \frac{3}{2}(\frac{1}{3})C + 2(\frac{3}{4})(\frac{7}{3}) + \frac{3}{2}(\frac{1}{3})(2) = 0$

These six equations can be simplified as $\ldots\ldots\ldots\ldots$

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On A	$B/2+D=13/4$
On B	$-A+C+E=10/4$
On C	$-3B/2+F=-5/4$
On D	$-A/2+E/2=0$
On E	$-B/2-D+F=-1$
On F	$-C/2-3E/2=-9/2$

These six simultaneous linear equations can be expressed in matrix form as ....

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$$\begin{pmatrix} 0 & 0{\cdot}5 & 0 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 & 1 & 0 \\ 0 & -1{\cdot}5 & 0 & 0 & 0 & 1 \\ -0{\cdot}5 & 0 & 0 & 0 & 0{\cdot}5 & 0 \\ 0 & -0{\cdot}5 & 0 & -1 & 0 & 1 \\ 0 & 0 & -0{\cdot}5 & 0 & -1{\cdot}5 & 0 \end{pmatrix}\begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 13/4 \\ 10/4 \\ -5/4 \\ 0 \\ -1 \\ -9/2 \end{pmatrix}$$

That is

$\mathbf{Ax} = \mathbf{b}$ with solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$

Inverting the matrix $\mathbf{A}$ we find that

$$\begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 2{\cdot}166\ldots \\ 2{\cdot}3\ldots \\ 2{\cdot}5 \\ 2{\cdot}0833\ldots \\ 2{\cdot}166\ldots \\ 2{\cdot}25 \end{pmatrix} = \begin{pmatrix} 13/6 \\ 7/3 \\ 5/2 \\ 25/12 \\ 13/6 \\ 9/4 \end{pmatrix}$$

which is identical to the values found from the exact solution $f(x, y) = xy + 2$.

Next frame

Derivative boundary conditions

20

The process of solving a differential equation, either ordinary or partial, involves using indefinite integration and each time we integrate we produce an integration constant. For a differential equation to have a complete solution, where all the integration constants are evaluated, the differential equation must be accompanied by a set of conditions that are sufficient to do this.

If the differential equation involves time t then it is natural for these ▶

conditions to give values of the function and its derivatives at time $t = 0$. Such conditions are known as *initial conditions* and we have met these before when we studied the Laplace transform, for example. Other conditions, like the conditions we met in the previous two examples, are called *boundary conditions* because they gave the values of the function on the boundary of the function domain. We now consider boundary conditions in the form of derivatives normal to the boundary and this we do in the following example.

Example 3

Find the solution to $4\dfrac{\partial f(x,y)}{\partial x} + 2\dfrac{\partial f(x,y)}{\partial y} = 3$, for $0 \le x \le 1$ and $0 \le y \le 1$ given that the boundary conditions are

$$f(x,0) = f(x,1) = f(0,y) = 10$$

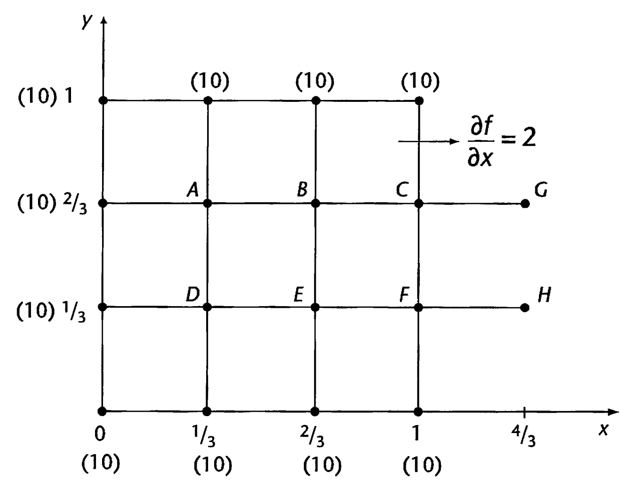
and $$\left.\frac{\partial f(x,y)}{\partial x}\right|_{x=1} = 2$$

for a mesh of size $1/3$ in both the x-direction and the y-direction.

Next frame

21

The domain of $f(x, y)$ is the square of side length 1 as shown in the diagram:



Overlaid on the function domain in the x–y plane is a mesh of grid points. Because the boundary condition relating to the side $x = 1$ is in the form of a derivative normal to the side, *we extend the grid over the boundary of the function domain by adding two additional points outside the domain* and distant $1/3$ from it, as shown in the figure.

The values of $f(x, y)$ that we can compute from the boundary conditions alone are shown in brackets. The values of $f(x, y)$ that we have to determine are labelled A to F and we shall need the two additional points G and H outside the domain of $f(x, y)$ to do this. ▶

The second part of the procedure is to find the central difference formula that describes the differential equation:

We have $\left.\dfrac{\partial f(x, y)}{\partial x}\right|_{ij} = \dfrac{f_{i+1,j} - f_{i-1,j}}{2h} = 1{\cdot}5\left(f_{i+1,j} - f_{i-1,j}\right)$

$$\left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = \frac{f_{i,j+1} - f_{i,j-1}}{2k} = 1{\cdot}5\left(f_{i,j+1} - f_{i,j-1}\right)$$

because both h and $k = 1/3$

Therefore

$$4\frac{\partial f(x, y)}{\partial x} + 2\frac{\partial f(x, y)}{\partial y} = 3 \text{ becomes } \ldots\ldots\ldots\ldots$$

22

$$\boxed{6\left(f_{i+1,j} - f_{i-1,j}\right) + 3\left(f_{i,j+1} - f_{i,j-1}\right) = 3}$$

Because

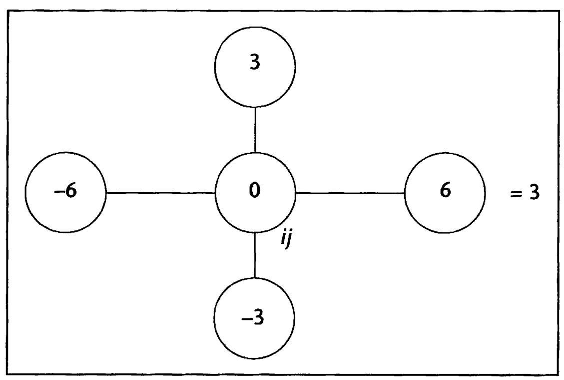
$4\dfrac{\partial f(x, y)}{\partial x} + 2\dfrac{\partial f(x, y)}{\partial y} = 3$ can be written as

$4 \times 1{\cdot}5\left(f_{i+1,j} - f_{i-1,j}\right) + 2 \times 1{\cdot}5\left(f_{i,j+1} - f_{i,j-1}\right) = 3$, that is

$6\left(f_{i+1,j} - f_{i-1,j}\right) + 3\left(f_{i,j+1} - f_{i,j-1}\right) = 3$

This has the computational molecule ....

23



We now place the centre of the molecule, in turn, on each of the grid points that we need to evaluate:

On A $-60 + 30 + 6B - 3E = 3$

On B $-6A + 30 + 6C - 3E = 3$

On C ....

On D ....

On E ....

On F ....

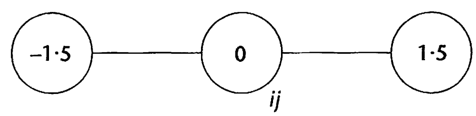
24

On A	$-60+30+6B-3E=3$
On B	$-6A+30+6C-3E=3$
On C	$-6B+30+6G-3F=3$
On D	$-60+3A+6E-30=3$
On E	$-6D+3B+6F-30=3$
On F	$-6E+3C+6H-30=3$

At the boundary $x=1$ the boundary condition $\left.\dfrac{\partial f(x,y)}{\partial x}\right|_{x=1}=2$ can be written using the central difference formula as

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{\substack{x=1\\y=y_j}}=\frac{f_{i+1,j}-f_{i-1,j}}{2h}=1{\cdot}5(f_{i+1,j}-f_{i-1,j})=2$$

which has the computational molecule:



We now place the centre of this molecule, in turn, on each of the grid points C and F to obtain

On C $-1{\cdot}5B+1{\cdot}5G=2$

On F . . . .

25

On C	$-1{\cdot}5B+1{\cdot}5G=2$
On F	$-1{\cdot}5E+1{\cdot}5H=2$

We can now use these last two equations either to eliminate the points G and H from the six equations in Frame 24 or to form an 8×8 system. We shall eliminate the points G and H to obtain the six equations, with the constant on the right-hand side as

. . . .

26

On A	$6B-3E=33$
On B	$-6A+6C-3E=-27$
On C	$-3F=-35$
On D	$3A+6E=93$
On E	$-6D+3B+6F=33$
On F	$3C=25$

These six simultaneous linear equations can be expressed in matrix form as . . . .

27

$$\begin{pmatrix} 0 & 6 & 0 & 0 & -3 & 0 \\ -6 & 0 & 6 & 0 & -3 & 0 \\ 0 & 0 & 0 & 0 & 0 & -3 \\ 3 & 0 & 0 & 0 & 6 & 0 \\ 0 & 3 & 0 & -6 & 0 & 6 \\ 0 & 0 & 3 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 33 \\ -27 \\ -35 \\ 93 \\ 33 \\ 25 \end{pmatrix}$$

That is

$\mathbf{Ax} = \mathbf{b}$ with solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$

Inverting the matrix $\mathbf{A}^{-1}$ we find that $\mathbf{x} =$ ....

28

$$\begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 6{\cdot}777\ldots \\ 11{\cdot}555\ldots \\ 8{\cdot}333\ldots \\ 11{\cdot}9444\ldots \\ 12{\cdot}111\ldots \\ 11{\cdot}666\ \ldots \end{pmatrix} = \begin{pmatrix} 61/9 \\ 104/9 \\ 25/3 \\ 215/18 \\ 109/9 \\ 35/3 \end{pmatrix}$$

Next frame

Second-order partial differential equations

29

The most general form of a second-order partial differential equation is

$$a(x,y)\frac{\partial^2 f}{\partial x^2} + b(x,y)\frac{\partial^2 f}{\partial x \partial y} + c(x,y)\frac{\partial^2 f}{\partial y^2} + d(x,y)\frac{\partial f}{\partial x} + e(x,y)\frac{\partial f}{\partial y} + g(x,y) = 0$$

Three types of equation are of particular interest because they feature so prominently in engineering and science.

Elliptic equations

If $b^2 - 4ac < 0$ the partial differential equation is called an *elliptic* equation. Such equations arise out of steady-state problems as occur in potential or flow theory. Two examples are

Poisson's equation

$$\frac{\partial^2\phi(x,y)}{\partial x^2} + \frac{\partial^2\phi(x,y)}{\partial y^2} = g(x,y)$$

Laplace's equation

$$\frac{\partial^2\phi(x,y)}{\partial x^2} + \frac{\partial^2\phi(x,y)}{\partial y^2} = 0$$

In both cases $a = 1$, $b = 0$ and $c = 1$ and so $b^2 - 4ac < -4$.

▶

Hyperbolic equations

If $b^2 - 4ac > 0$ the partial differential equation is called an *hyperbolic* equation. Such equations arise out of vibrational and radiative problems as occur in wave mechanics. An example is

The wave equation

$$\frac{\partial^2 \phi(x,t)}{\partial x^2} = \frac{1}{\kappa^2}\frac{\partial^2 \phi(x,t)}{\partial t^2}$$

Here $a = 1$, $b = 0$ and $c = -\dfrac{1}{\kappa^2}$ and so $b^2 - 4ac > 0$.

Parabolic equations

If $b^2 - 4ac = 0$ the partial differential equation is called a *parabolic* equation. Such equations arise out of transient flow problems as occur in conduction or consolidation. An example is

The consolidation (or heat conduction) equation

$$\frac{\partial^2 \phi(x,t)}{\partial x^2} = \frac{1}{\kappa}\frac{\partial \phi(x,t)}{\partial t}$$

Here $a = 1$, $b = 0$ and $c = 0$ and so $b^2 - 4ac = 0$.

In the equations above a, b and c are constant but in the general case they depend on x and y and so a given equation may change from one type to another within the same domain.

Next frame

Second partial derivatives

30

In Frame 4 we found that for a function of a single real variable $f(x)$ the central difference formula approximating the second derivative was

$$f''(x) \approx \frac{f(x-h) - 2f(x) + f(x+h)}{h^2}$$

The second derivative at x is given as the sum of the two adjacent values less twice the value at the point, all divided by h^2.

If we apply this to a function of two real variables $f(x, y)$ and use $f_{i,j} \equiv f(ih, jk)$ to represent the value of $f(x, y)$ at the point (ih, jk) then the central difference formulas for the second partial derivatives with respect to x and y are seen to be ....

31

$$\boxed{\begin{aligned} \left.\frac{\partial^2 f(x,y)}{\partial x^2}\right|_{ij} &\approx \frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{h^2} \\ \left.\frac{\partial^2 f(x,y)}{\partial y^2}\right|_{ij} &\approx \frac{f_{i,j-1} - 2f_{i,j} + f_{i,j+1}}{k^2} \end{aligned}}$$

Because

The second derivative at x_i is given as the sum of the two adjacent values on the jth row less twice the value at x_i, all divided by the cell width squared – h^2, and so

$$\left.\frac{\partial^2 f(x,y)}{\partial x^2}\right|_{ij} \approx \frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{h^2}$$

The second derivative at y_j is given as the sum of the two adjacent values in the jth column less twice the value at y_j, all divided by the cell height squared – k^2, and so

$$\left.\frac{\partial^2 f(x,y)}{\partial y^2}\right|_{ij} \approx \frac{f_{i,j-1} - 2f_{i,j} + f_{i,j+1}}{k^2}$$

We are now ready to consider the construction of central difference formulas for second-order partial differential equations. We shall proceed by example.

Example 4

Given a grid with mesh size $h = k = 1/3$, find a numerical solution to the equation

$$\frac{\partial^2 f(x,y)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial y^2} = 0 \text{ for } 0 \leq x \leq 1,\ 0 \leq y \leq 1, \text{ given that}$$

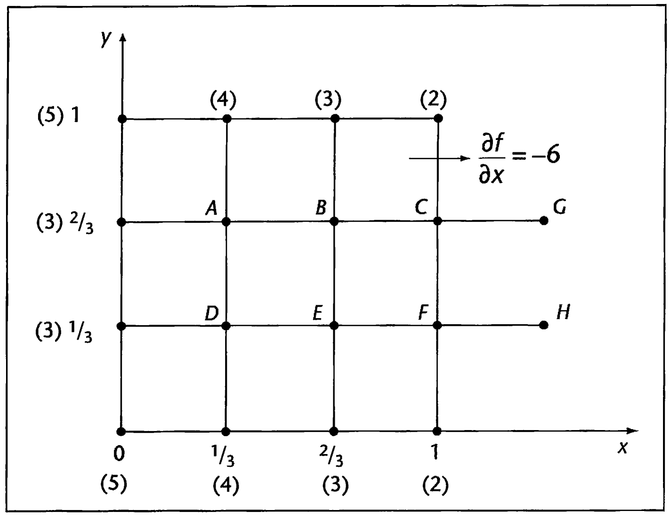
$$f(x,0) = f(x,1) = 5 - 3x$$

$$f(0,y) = 9y^2 - 9y + 5 \quad \text{and}$$

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{x=1} = -6$$

The domain with the grid overlaid is ....

32



The solution is to be evaluated at the grid points A to F – the external grid points G and H are inserted to accommodate the derivative boundary condition. The numbers in brackets are the values of $f(x, y)$ as found from the boundary conditions.

The central difference formula that represents the partial differential equation is ....

33

$$\boxed{9\left(f_{i+1,j} + f_{i,j+1} - 4f_{i,j} + f_{i-1,j} + f_{i,j-1}\right)}$$

Because

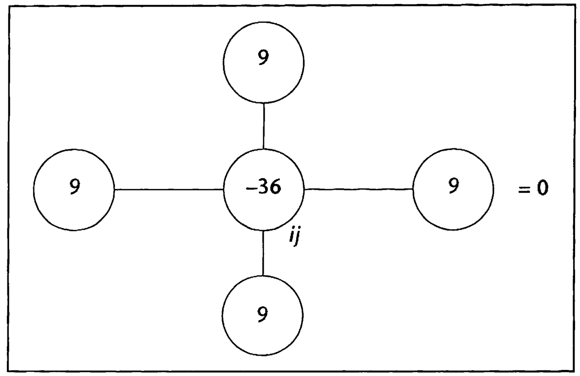
$$\left.\frac{\partial^2 f(x, y)}{\partial x^2}\right|_{ij} + \left.\frac{\partial^2 f(x, y)}{\partial y^2}\right|_{ij} \approx \frac{f_{i+1,j} - 2f_{i,j} + f_{i-1,j}}{h^2} + \frac{f_{i,j+1} - 2f_{i,j} + f_{i,j-1}}{k^2}$$

$$= 9\left(f_{i+1,j} - 2f_{i,j} + f_{i-1,j}\right) + 9\left(f_{i,j+1} - 2f_{i,j} + f_{i,j-1}\right)$$

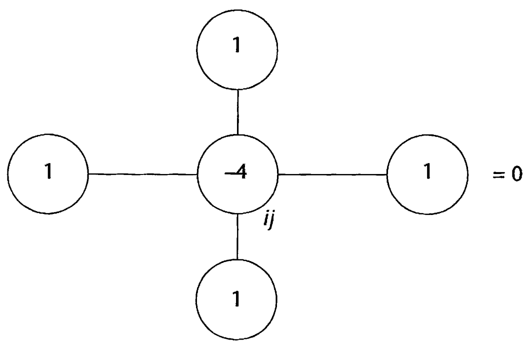
$$= 9\left(f_{i+1,j} + f_{i,j+1} - 4f_{i,j} + f_{i-1,j} + f_{i,j-1}\right)$$

From this we can construct the computational molecule for this differential equation as ....

34



If we applied this computational molecule to the grid points A to F then the six simultaneous linear equations that result would all have a common factor of 9 arising from the 9 in the molecule. If we divided every equation by 9 to remove this common factor we would not change the overall validity of the equations. So, to make the computation simpler we divide each term in the computational molecule by 9 and use the resulting molecule:



We now proceed as we have done before. Laying the centre of the computational molecule on each grid point in turn gives the six simultaneous linear equations:

At *A* $3+4+B+D-4A=0$
At *B* ....
At *C* ....
At *D* ....
At *E* ....
At *F* ....

35

At A	$3+4+B+D-4A=0$
At B	$A+3+C+E-4B=0$
At C	$B+2+G+F-4C=0$
At D	$3+A+E+4-4D=0$
At E	$D+B+F+3-4E=0$
At F	$E+C+H+2-4F=0$

We now apply the derivative boundary condition at the grid points C and F by using the computational molecule for the first partial derivative with respect to x

$$\left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = \frac{f_{i+1,j} - f_{i-1,j}}{2h} = \frac{3}{2}(f_{i+1,j} - f_{i-1,j}) = -6$$

This gives ....

36

$$\frac{3}{2}(-B+G) = -6$$
$$\frac{3}{2}(-E+H) = -6$$

Because

The computational molecule for the first partial derivative with respect to x is

$$\left.\frac{\partial f(x, y)}{\partial x}\right|_{ij} = \frac{-f_{i-1,j} + f_{i+1,j}}{2h} = \frac{3}{2}(-f_{i-1,j} + f_{i+1,j}) \text{ because } h = 1/3$$

Applying this molecule at the boundary points C and F gives the two equations

$$\frac{3}{2}(-B+G) = -6 \text{ so } G = -4+B$$
$$\frac{3}{2}(-E+H) = -6 \text{ so } H = -4+E$$

Substitution of these two equations into the first six eliminates the grid points G and H to produce the six equations in six unknowns.

These are written in matrix form as ....

37

$$\begin{pmatrix} -4 & 1 & 0 & 1 & 0 & 0 \\ 1 & -4 & 1 & 0 & 1 & 0 \\ 0 & 2 & -4 & 0 & 0 & 1 \\ 1 & 0 & 0 & -4 & 1 & 0 \\ 0 & 1 & 0 & 1 & -4 & 1 \\ 0 & 0 & 1 & 0 & 2 & -4 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} -7 \\ -3 \\ 2 \\ -7 \\ -3 \\ 2 \end{pmatrix}$$

which has solution ....

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$$\begin{pmatrix} A \\ B \\ C \\ D \\ E \\ F \end{pmatrix} = \begin{pmatrix} 28/9 \\ 7/3 \\ 8/9 \\ 28/9 \\ 7/3 \\ 8/9 \end{pmatrix}$$

Next frame

Time-dependent equations

39

Many physical systems have their behaviour modelled by a differential equation. For example, a long thin metal bar of length L, insulated along its length, has its ends maintained at a temperature of 0°C and, at time $t = 0$, the temperature distribution is given by

$$T(x, 0) = x^2 - 2xL + L^2$$

The future distribution of temperature $T(x, t)$ can then be found by solving the partial differential equation (the *heat equation*)

$$\frac{\partial^2 T(x, t)}{\partial x^2} = \frac{1}{\kappa}\frac{\partial T(x, t)}{\partial t}$$

subject to the given boundary and initial conditions. The constant $\kappa = \dfrac{K}{\omega}$ is called the *diffusivity* constant where K is the *thermal conductivity* and ω is the *specific heat per unit volume* of the metal that constitutes the rod. Apart from the physical considerations that set up the equation in the first place, the dimensions of κ are $[L^2T^{-1}]$ and are necessary to balance the dimensions on either side of the equation.

If we wished to solve the heat equation numerically as it stands then we would need to know the value of κ, and this would vary depending upon the specific metal used for the bar. We can overcome this problem by absorbing κ using a process of *dimension analysis* when we transform the equation into an equation of the form

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

where the variables x and t are now dimensionless – they are measured in numbers rather than units of distance and time respectively. How this is done we shall leave to the end of the Programme. For now we are interested in numerically solving such dimensionless equations over a rectangular domain of width 1, and as usual we shall proceed by example.

Next frame

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Example 5

Solve the partial differential equation

$$\frac{\partial^2 f(x,t)}{\partial x^2} = \frac{\partial f(x,t)}{\partial t}$$

for $0 \leq x \leq 1$ and $t \geq 0$ where

$$f(0,t) = 1$$
$$f(x,0) = 1 + x \text{ and}$$
$$\left.\frac{\partial f(x,t)}{\partial x}\right|_{x=1} = 0$$

We now have a change in procedure. Hitherto, the first thing we did was to draw the domain of the function with the grid overlaid. We could do this because we knew the step lengths in the x- and y-directions from the beginning. Here, the first thing we must do is to construct the finite difference formula that will represent the differential equation because its structure will dictate the step lengths. We can immediately write down the central difference formula for the second derivative on the left of this equation.

It is ....

41

$$\boxed{\left.\frac{\partial^2 f(x,t)}{\partial x^2}\right|_{ij} \approx \frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{h^2}}$$

To use a central difference formula for the derivative with respect to t would require a knowledge of $f(x, t)$ for values of $t < 0$ and this we do not possess. Consequently, for the derivative with respect to t we use the *forward* difference formula. Do you remember this one?

It is ....

42

$$\boxed{\left.\frac{\partial f(x,t)}{\partial t}\right|_{ij} \approx \frac{f_{i,j+1} - f_{i,j}}{k}}$$

Because

For a function of a single real variable the forward difference formula is given as

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \text{ and so } \left.\frac{\partial f(x,t)}{\partial t}\right|_{ij} \approx \frac{f_{i,j+1} - f_{i,j}}{k}$$

Using these two finite difference formulas we can write down the finite difference representation of the partial differential equation.

The finite difference representation is ....

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$$\boxed{\frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{h^2} = \frac{f_{i,j+1} - f_{i,j}}{k}}$$

That is

$$f_{i,j+1} = f_{i,j} + \frac{k}{h^2}(f_{i-1,j} - 2f_{i,j} + f_{i+1,j})$$

It can be shown that there will be no growth of rounding errors when evaluating this equation if $\frac{k}{h^2} \leq \frac{1}{2}$.

In compliance with this condition we shall take $h = 0{\cdot}2$ and $k = 0{\cdot}02$ so that $\frac{k}{h^2} = \frac{1}{2}$. We shall also restrict ourselves to finding solutions for t ranging from 0 to 0·16.

The finite difference equation then reduces to ....

44

$$\boxed{f_{i,j+1} = \frac{1}{2}(f_{i-1,j} + f_{i+1,j})}$$

Because

$$f_{i,j+1} = f_{i,j} + \frac{k}{h^2}(f_{i-1,j} - 2f_{i,j} + f_{i+1,j}) \text{ and so}$$

$$f_{i,j+1} = f_{i,j} + \frac{1}{2}(f_{i-1,j} - 2f_{i,j} + f_{i+1,j}) = \frac{1}{2}(f_{i-1,j} + f_{i+1,j})$$

Notice that this is an equation for stepping forwards in time, so that given the solution is known at $t = 0$ then the solution at $t = k$ can be found from this equation. We can use our spreadsheet to construct the solution from this equation. Open your spreadsheet and

1 Cell A1 enter ***t*** \ ***x*** to represent the fact that the first column will contain the t-values and the first row the x-values.

2 In cells B1 to H1 enter the values of x from 0 to 1·2 in steps of 0·2.

The column headed 1·2 contains grid points outside the domain of $f(x, t)$ to accommodate the derivative boundary condition.

3 In cells A2 to A10 enter the values of t from 0 to 0·16 in steps of 0·02.

4 In cells B2 to B10 enter the value 1 to represent the boundary condition $f(0, t) = 1$.

5 In cell C2 enter the formula **=1+C1** to represent the initial condition $f(x, 0) = 1 + x$. Copy this formula into cells D2 to G2.

6 In cell C3 enter the formula **=0·5*(B2+D2)** to represent the finite difference equation

$$f_{i,j+1} = \frac{1}{2}(f_{i-1,j} + f_{i+1,j})$$

▶

7 Copy the contents of cell C3 into the block of cells C3 to G10.

Because the derivative boundary condition $\left.\dfrac{\partial f(x, t)}{\partial x}\right|_{x=1} = 0$ is represented by the central difference formula $f_{i+1,j} - f_{i-1,j} = 0$, the values of $f(x, t)$ at the external grid points when $x = 1{\cdot}2$ are equal to the values at the internal grid points when $x = 0{\cdot}8$.

8 In cell H2 enter the formula **=F2** and copy this into cells H3 to H10 to produce the following final display:

$t\backslash x$	0·0	0·2	0·4	0·6	0·8	1·0	1·2
0·00	1·00000	1·20000	1·40000	1·60000	1·80000	2·00000	1·80000
0·02	1·00000	1·20000	1·40000	1·60000	1·80000	1·80000	1·80000
0·04	1·00000	1·20000	1·40000	1·60000	1·70000	1·80000	1·70000
0·06	1·00000	1·20000	1·40000	1·55000	1·70000	1·70000	1·70000
0·08	1·00000	1·20000	1·37500	1·55000	1·62500	1·70000	1·62500
0·10	1·00000	1·18750	1·37500	1·50000	1·62500	1·62500	1·62500
0·12	1·00000	1·18750	1·34375	1·50000	1·56250	1·62500	1·56250
0·14	1·00000	1·17188	1·34375	1·45313	1·56250	1·56250	1·56250
0·16	1·00000	1·17188	1·31250	1·45313	1·50781	1·56250	1·50781

If the diffusion equation in Frame 40 to which this solution refers is taken to represent the temperature distribution along a heated rod then this tableau displays how the temperature is changing both in time and spatially along the rod. Notice how, as the heat diffuses through the rod, the temperature changes faster at points that are further away from the end that is maintained at constant temperature.

Try one yourself. Next frame

45

Example 6

The solution of the partial differential equation

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \le x \le 1$ taken in steps of $h = 0{\cdot}2$ and $0 \le t \le 0{\cdot}16$ in steps of $k = 0{\cdot}02$ where

$$f(0, t) = 2$$

$$f(x, 0) = 2 + x \quad \text{and} \quad \left.\frac{\partial f(x, t)}{\partial x}\right|_{x=1} = 0{\cdot}5$$

is ....

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$t \backslash x$	0·0	0·2	0·4	0·6	0·8	1·0	1·2
0·00	2·00000	2·20000	2·40000	2·60000	2·80000	3·00000	3·00000
0·02	2·00000	2·20000	2·40000	2·60000	2·80000	2·90000	3·00000
0·04	2·00000	2·20000	2·40000	2·60000	2·75000	2·90000	2·95000
0·06	2·00000	2·20000	2·40000	2·57500	2·75000	2·85000	2·95000
0·08	2·00000	2·20000	2·38750	2·57500	2·71250	2·85000	2·91250
0·10	2·00000	2·19375	2·38750	2·55000	2·71250	2·81250	2·91250
0·12	2·00000	2·19375	2·37188	2·55000	2·68125	2·81250	2·88125
0·14	2·00000	2·18594	2·37188	2·52656	2·68125	2·78125	2·88125
0·16	2·00000	2·18594	2·35625	2·52656	2·65391	2·78125	2·85391

Because

$$f_{i,j+1} = f_{i,j} + \frac{k}{h^2}\left(f_{i-1,j} - 2f_{i,j} + f_{i+1,j}\right) \text{ and so}$$

$$f_{i,j+1} = f_{i,j} + \frac{1}{2}\left(f_{i-1,j} - 2f_{i,j} + f_{i+1,j}\right) = \frac{1}{2}\left(f_{i-1,j} + f_{i+1,j}\right)$$

We can use our spreadsheet to construct the solution from this equation. Open your spreadsheet and

1. In cell A1 enter **$t \backslash x$** to represent the fact that the first column will contain the t-values and the first row the x-values.
2. In cells B1 to H1 enter the values of x from 0 to 1·2 in steps of 0·2.

The column headed 1·2 contains grid points outside the domain of $f(x, t)$ to accommodate the derivative boundary condition.

3. In cells A2 to A10 enter the values of t from 0 to 0·16 in steps of 0·02.
4. In cells B2 to B10 enter the value 2 to represent the boundary condition $f(0, t) = 2$.
5. In cell C2 enter the formula **=2+C1** to represent the initial condition $f(x, 0) = 2 + x$. Copy this formula into cells D2 to G2.
6. In cell C3 enter the formula to represent the finite difference equation

   $$f_{i,j+1} = \frac{1}{2}\left(f_{i-1,j} + f_{i+1,j}\right)$$

   The formula is ....

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=0.5*(B2+D2)

7 Copy the contents of cell C3 into the block of cells C3 to G10.

Because the derivative boundary condition $\left.\dfrac{\partial f(x, t)}{\partial x}\right|_{x=1} = 0{\cdot}5$ is represented by the central difference formula $f_{i+1,j} - f_{i-1,j} = 0{\cdot}2$, the values of $f(x, t)$ at the external grid points when $x = 1{\cdot}2$ are equal to

The values at the internal grid points when
$x =$ .... plus ....

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$x = 0{\cdot}8$ plus $0{\cdot}2$

8 In cell H2 enter the formula **=F2+0·2** and copy this into cells H3 to H10 to produce the following display:

t\x	0·0	0·2	0·4	0·6	0·8	1·0	1·2
0·00	2·00000	2·20000	2·40000	2·60000	2·80000	3·00000	3·00000
0·02	2·00000	2·20000	2·40000	2·60000	2·80000	2·90000	3·00000
0·04	2·00000	2·20000	2·40000	2·60000	2·75000	2·90000	2·95000
0·06	2·00000	2·20000	2·40000	2·57500	2·75000	2·85000	2·95000
0·08	2·00000	2·20000	2·38750	2·57500	2·71250	2·85000	2·91250
0·10	2·00000	2·19375	2·38750	2·55000	2·71250	2·81250	2·91250
0·12	2·00000	2·19375	2·37188	2·55000	2·68125	2·81250	2·88125
0·14	2·00000	2·18594	2·37188	2·52656	2·68125	2·78125	2·88125
0·16	2·00000	2·18594	2·35625	2·52656	2·65391	2·78125	2·85391

The Crank–Nicolson procedure

The forward difference formula that we used for the derivative with respect to time is not as accurate as a central difference formula. However, because we do not possess information about $f(x, t)$ for $t < 0$ we were forced to adopt the forward difference formula. To overcome this the Crank–Nicolson procedure makes the assumption that the partial differential equation is satisfied not just at the grid points but also at points in time halfway between two grid points. That is 49

$$\left.\frac{\partial^2 f(x, t)}{\partial x^2}\right|_{i,j+1/2} = \left.\frac{\partial f(x, t)}{\partial t}\right|_{i,j+1/2}$$

▶

We can then derive a central finite difference formula for the time derivative based on this intermediate point

$$\left.\frac{\partial f(x,\,t)}{\partial t}\right|_{i,j+1/2}=\frac{f_{i,j+1}-f_{i,j}}{2(k/2)}=\frac{f_{i,j+1}-f_{i,j}}{k}$$

Here the two grid points either side of the $i,\, j+1/2$th point are the $i,\, j$th and the $i,\, j+1$th, each separated by half the grid step in the time direction. You will note that the outcome is identical to the forward difference taken from the $i,\, j$th grid point. However, the finite difference formula that represents the partial differential equation will *not* be the same. For the second derivative with respect to x on the left-hand side of the equation we use a finite difference formula that is the average of the central difference formulas for the i, jth grid point and the $i, j+1$th grid point. That is

$$\left.\frac{\partial^2 f(x,\,t)}{\partial x^2}\right|_{i,j+1/2}=\frac{1}{2}\left(\frac{f_{i-1,j}-2f_{i,j}+f_{i+1,j}}{h^2}+\frac{f_{i-1,j+1}-2f_{i,j+1}+f_{i+1,j+1}}{h^2}\right)$$

The partial differential equation is then represented by the central difference formula ....

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$$\boxed{\frac{1}{2}\left(\frac{f_{i-1,j}-2f_{i,j}+f_{i+1,j}}{h^2}+\frac{f_{i-1,j+1}-2f_{i,j+1}+f_{i+1,j+1}}{h^2}\right)=\frac{f_{i,j+1}-f_{i,j}}{k}}$$

That is

$$\begin{aligned}&-f_{i,j+1}+\frac{k}{2h^2}\left(f_{i-1,j+1}-2f_{i,j+1}+f_{i+1,j+1}\right)\\&\quad=-f_{i,j}-\frac{k}{2h^2}\left(f_{i-1,j}-2f_{i,j}+f_{i+1,j}\right)\end{aligned}$$

Unlike the previous case there is now no restriction on the value of $\dfrac{k}{2h^2}$ and different choices of h and k will result in different difference formulas. If we choose $\dfrac{k}{2h^2}=1$ this difference formula becomes

$$f_{i-1,j+1}-3f_{i,j+1}+f_{i+1,j+1}=-f_{i-1,j}+f_{i,j}-f_{i+1,j}$$

So we have three unknown quantities on the left-hand side of this equation given in terms of three known quantities on the right. We shall do an example to see exactly how this procedure operates.

Next frame

Example 7

Use the Crank–Nicolson procedure to solve the partial differential equation

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \le x \le 1$ taken in steps of $h = 0{\cdot}25$ and $0 \le t \le 0{\cdot}5$ in steps of $k = 0{\cdot}125$ where:

$$f(0, t) = f(1, t) = 0$$
$$f(x, 0) = x(1 - x)$$

We can use our spreadsheet to construct the solution from this equation. Open your spreadsheet and

1 In cell A1 enter ***t* \ *x*** to represent the fact that the first column will contain the t-values and the first row the x-values.
2 In cells B1 to F1 enter the values of x from 0 to 1 in steps of 0·25.
3 In cells A2 to A6 enter the values of t from 0 to 0·5 in steps of 0·125.
4 In cells B2 to B6 enter the value 0 to represent the boundary condition $f(0, t) = 0$.
5 In cells F2 to F6 enter the value 0 to represent the boundary condition $f(1, t) = 0$.
6 In cell C2 enter the formula **=C1*(1−C1)** to represent the boundary condition $f(x, 0) = x(1 - x)$ and copy into cells D2 to F2.

We now want to know the values that are going to go into the block of cells C3 to E6. We shall work on one row at a time and consider cells C3, D3 and E3 – we shall call these values A, B and C respectively.

Applying the central difference formula for the differential equation

$$f_{i-1,j+1} - 3f_{i,j+1} + f_{i+1,j+1} = -f_{i-1,j} + f_{i,j} - f_{i+1,j}$$

we find that by working along rows 2 and 3

From columns B to D: $0 - 3A + B = -0 + 0{\cdot}1875 - 0{\cdot}25$, that is $-3A + B = -0{\cdot}0625$

From columns C to E: $A - 3B + C = -0{\cdot}1875 + 0{\cdot}25 - 0{\cdot}1875$, that is $A - 3B + C = -0{\cdot}125$

From columns D to F: $B - 3C + 0 = -0{\cdot}25 + 0{\cdot}1875 - 0$, that is $B - 3C = -0{\cdot}0625$

These equations have solution

$A = 0{\cdot}044643$, $B = 0{\cdot}071429$ and $C = 0{\cdot}044643$

Enter these values into cells C3 to E3 respectively and repeat the procedure to find the values in cells C4 to E4.

These are C4: ...., D4: .... and E4: ....

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C4: 0·014031, D4: 0·015306 and E4: 0·014031

Because

From columns B to D: $-3A + B = -0{\cdot}026786$

From columns C to E: $A - 3B + C = -0{\cdot}017857$

From columns D to F: $B - 3C = -0{\cdot}026786$

These equations have solution

$A = 0{\cdot}014031$, $B = 0{\cdot}015306$ and $C = 0{\cdot}014031$

This process is repeated until all the appropriate values have been found, giving the following display:

t\x	0·00	0·25	0·50	0·75	1·00
0·000	0·000000	0·187500	0·250000	0·187500	0·000000
0·125	0·000000	0·044643	0·071429	0·044643	0·000000
0·250	0·000000	0·014031	0·015306	0·014031	0·000000
0·375	0·000000	0·002369	0·005831	0·002369	0·000000
0·500	0·000000	0·001328	0·000521	0·001328	0·000000

Try one yourself.

Next frame

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Example 8

Use the Crank–Nicolson procedure to solve the partial differential equation

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \le x \le 1$ taken in steps of $h = 0{\cdot}2$ and $0 \le t \le 0{\cdot}2$ in steps of $k = 0{\cdot}04$ where

$f(0, t) = 2$

$f(1, t) = 1$

$f(x, 0) = 2 - x^2$

The very first thing we must do in solving this equation numerically is ....

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Derive the finite difference equation to be used

Because

The Crank–Nicolson procedure tells us that

$$-f_{i,j+1}+\frac{k}{2h^2}\left(f_{i-1,j+1}-2f_{i,j+1}+f_{i+1,j+1}\right)$$
$$=-f_{i,j}-\frac{k}{2h^2}\left(f_{i-1,j}-2f_{i,j}+f_{i+1,j}\right)$$

so for each different ratio $\frac{k}{2h^2}$ we have a different finite difference formula.

Here we choose $h=0{\cdot}2$ and $k=0{\cdot}04$ so that $\frac{k}{2h^2}=\frac{1}{2}$ and the terms in $f_{i,j}$ do not appear.

This gives the finite difference formula ....

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$$\boxed{f_{i-1,j+1}-4f_{i,j+1}+f_{i+1,j+1}=-\left(f_{i-1,j}+f_{i+1,j}\right)}$$

Because

$$-f_{i,j+1}+\frac{k}{2h^2}\left(f_{i-1,j+1}-2f_{i,j+1}+f_{i+1,j+1}\right)$$
$$=-f_{i,j}-\frac{k}{2h^2}\left(f_{i-1,j}-2f_{i,j}+f_{i+1,j}\right)$$

and so

$$-f_{i,j+1}+\frac{1}{2}\left(f_{i-1,j+1}-2f_{i,j+1}+f_{i+1,j+1}\right)=-f_{i,j}-\frac{1}{2}\left(f_{i-1,j}-2f_{i,j}+f_{i+1,j}\right)$$

that is

$$\frac{1}{2}\left(f_{i-1,j+1}-4f_{i,j+1}+f_{i+1,j+1}\right)=-\frac{1}{2}\left(f_{i-1,j}+f_{i+1,j}\right)$$

giving

$$\left(f_{i-1,j+1}-4f_{i,j+1}+f_{i+1,j+1}\right)=-\left(f_{i-1,j}+f_{i+1,j}\right)$$

The complete solution required is ....

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$t\backslash x$	0·00	0·20	0·40	0·60	0·80	1·00
0·000	2·000000	1·960000	1·840000	1·640000	1·360000	1·000000
0·040	2·000000	1·901818	1·767273	1·567273	1·301818	1·000000
0·080	2·000000	1·870083	1·713058	1·513058	1·270083	1·000000
0·120	2·000000	1·847483	1·676875	1·476875	1·247483	1·000000
0·160	2·000000	1·832271	1·65221	1·45221	1·232271	1·000000
0·200	2·000000	1·821919	1·635467	1·435467	1·221919	1·000000

Because

Using your spreadsheet to construct the solution from this equation

1. In cell A1 enter $t\backslash x$ to represent the fact that the first column will contain the t-values and the first row the x-values.
2. In cells B1 to G1 enter the values of x from 0 to 1 in steps of 0·2.
3. In cells A2 to A7 enter the values of t from 0 to 0·2 in steps of 0·04.
4. In cells B2 to B7 enter the value 2 to represent the boundary condition $f(0, t) = 2$.
5. In cells G2 to G7 enter the value 1 to represent the boundary condition $f(1, t) = 1$.
6. In cell C2 enter the formula **=2–C1^2** to represent the boundary condition $f(x, 0) = 2 - x^2$ and copy into cells D2 to F2.

We now want to know the values that are going to go into the block of cells C3 to F7. We shall work on one row at a time and consider cells C3, D3, E3 and F3 – we shall call these values A, B, C and D respectively.

Applying the central difference formula for the differential equation

$$f_{i-1,j+1} - 4f_{i,j+1} + f_{i+1,j+1} = -(f_{i-1,j} + f_{i+1,j})$$

Then by working along rows 2 and 3

From columns B to D: $2 - 4A + B = -2 - 1{\cdot}6$, that is

$-4A + B = -5{\cdot}6$

From columns C to E: ....

From columns D to F: ....

From columns E to G: ....

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From columns B to D:	$-4A + B = -5{\cdot}6$
From columns C to E:	$A - 4B + C = -3{\cdot}2$
From columns D to F:	$B - 4C + D = -2{\cdot}8$
From columns E to G:	$C - 4D = -3{\cdot}4$

Because

From columns B to D: $2 - 4A + B = -2 - 1{\cdot}6$, that is $-4A + B = -5{\cdot}6$

From columns C to E: $A - 4B + C = -1{\cdot}8 - 1{\cdot}4$, that is $A - 4B + C = -3{\cdot}2$

From columns D to F: $B - 4C + D = -1{\cdot}6 - 1{\cdot}2$, that is $B - 4C + D = -2{\cdot}8$

From columns E to G: $C - 4D + 1 = -1{\cdot}4 - 1{\cdot}0$, that is $C - 4D = -3{\cdot}4$

These equations have solution

$A = \ldots\ldots\ldots\ldots$, $B = \ldots\ldots\ldots\ldots$,
$C = \ldots\ldots\ldots\ldots$ and $D = \ldots\ldots\ldots\ldots$

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$$\boxed{\begin{aligned} A &= 1{\cdot}901818 \\ B &= 1{\cdot}767273 \\ C &= 1{\cdot}567273 \\ D &= 1{\cdot}301818 \end{aligned}}$$

Enter these values into cells C3 to F3 respectively and repeat the procedure to find the values for cells C4 to F4.

These are C4: ...., D4: ....,
E4: .... and F4: ....

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C4: 1·870083
D4: 1·713058
E4: 1·513058
F4: 1·270083

Continuing in this way we find the complete solution as:

$t\backslash x$	0·00	0·20	0·40	0·60	0·80	1·00
0·000	2·000000	1·960000	1·840000	1·640000	1·360000	1·000000
0·040	2·000000	1·901818	1·767273	1·567273	1·301818	1·000000
0·080	2·000000	1·870083	1·713058	1·513058	1·270083	1·000000
0·120	2·000000	1·847483	1·676875	1·476875	1·247483	1·000000
0·160	2·000000	1·832271	1·65221	1·45221	1·232271	1·000000
0·200	2·000000	1·821919	1·635467	1·435467	1·221919	1·000000

Next frame

Dimensional analysis

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The equation of Frame 39

$$\frac{\partial^2 T(x,t)}{\partial x^2} = \frac{1}{\kappa}\frac{\partial T(x,t)}{\partial t} \quad \text{for } 0 \le x \le L \text{ and } t \ge 0$$

models the temperature distribution $T(x, t)$ along a long thin metal bar of length L. Solutions of this equation will produce values for the temperature distant x along the rod $(0 \le x \le L)$ at time t. The dimensions of the left- and right-hand sides of this equation due to the derivatives are

$$\left[\frac{\partial^2}{\partial x^2}\right] \equiv [L^{-2}] \text{ and } \left[\frac{\partial}{\partial t}\right] \equiv [T^{-1}]$$

To ensure that the dimensions of the left-hand side are the same as the dimensions of the right-hand side we find that the dimensions of $\frac{1}{\kappa}$ are

$$\left[\frac{1}{\kappa}\right] \equiv [L^{-2}T]$$

This then ensures that the equation compares quantities with the same dimension. To solve this equation numerically would require a knowledge of the value of κ which would be different for different problems. To avoid this we transform the equation into a dimensionless form, so ensuring that the variables are measured in numbers and not in any particular dimensional units. We do this as on the following page. ▶

Define new dimensionless variables as: $X = \dfrac{x}{L}$ (so that $0 \le X \le 1$), $\tau = \dfrac{\kappa t}{L^2}$ and define

$$U(X, \tau) = T(x[X], t[\tau])$$

then

$$\frac{\partial T}{\partial t} = \frac{\mathrm{d}\tau}{\mathrm{d}t}\frac{\partial U}{\partial \tau} = \frac{\kappa}{L^2}\frac{\partial U}{\partial \tau} \quad \text{and}$$

$$\frac{\partial T}{\partial x} = \frac{\mathrm{d}X}{\mathrm{d}x}\frac{\partial U}{\partial X} = \frac{1}{L}\frac{\partial U}{\partial X}$$

therefore $$\frac{\partial^2 T}{\partial x^2} = \frac{\partial}{\partial x}\frac{\partial T}{\partial x} = \frac{\partial}{\partial x}\frac{1}{L}\frac{\partial U}{\partial X} = \frac{\mathrm{d}X}{\mathrm{d}x}\frac{1}{L}\frac{\partial^2 U}{\partial X^2} = \frac{1}{L^2}\frac{\partial^2 U}{\partial X^2}$$

This means that

$$\frac{\partial^2 T(x,t)}{\partial x^2} = \frac{1}{\kappa^2}\frac{\partial T(x,t)}{\partial t} \quad \text{becomes}$$

$$\frac{1}{L^2}\frac{\partial^2 U(X,\tau)}{\partial X^2} = \frac{1}{\kappa L^2}\frac{\kappa\,\partial U(X,\tau)}{\partial \tau} = \frac{1}{L^2}\frac{\partial U(X,\tau)}{\partial \tau}$$

so $$\frac{\partial^2 U(X,\tau)}{\partial X^2} = \frac{\partial U(X,\tau)}{\partial \tau}$$

is the required equation in dimensionless form.

This now completes the work for this Programme. Read through the **Revision summary** that follows and then check your understanding against the **Can You?** checklist. When you are satisified that you do understand the contents of the Programme, try the **Test exercises**. There are no tricks and you should find them quite straightforward. Finally there are some **Further problems** to give additional practice.

Revision summary 13 61

1 *Numerical approximation to derivatives of $f(x)$*

The *forward difference formula*

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \quad \text{neglecting terms of the order } h$$

The *backward difference formula*

$$f'(x) \approx \frac{f(x) - f(x-h)}{h} \quad \text{neglecting terms of the order } h$$

The *central difference formulas*

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h} \quad \text{neglecting terms of the order } h^2$$

$$f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \quad \text{neglecting terms of the order } h^2.$$

2 *Functions of two real variables*

If $f(x, y)$ is single-valued, then to every domain point (x, y) there corresponds a single range point $f(x, y)$.

Grid values

The rectangular domain of the function is overlaid by a grid whose mesh size is of h units in the x-direction and k units in the y-direction. The value of $f(x, y)$ at the ijth grid point is denoted by

$$f_{i,j} \equiv f(x_0 + ih, y_0 + jk)$$

The values of the expression $f(x, y)$ are required to be found at the grid points

$$\begin{array}{ccccc} \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & f_{i-1,j+1} & f_{i,j+1} & f_{i+1,j+1} & \cdots \\ \cdots & f_{i-1,j} & f_{i,j} & f_{i+1,j} & \cdots \\ \cdots & f_{i-1,j-1} & f_{i,j-1} & f_{i+1,j-1} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \end{array}$$

3 *Central difference formulas for partial derivatives*

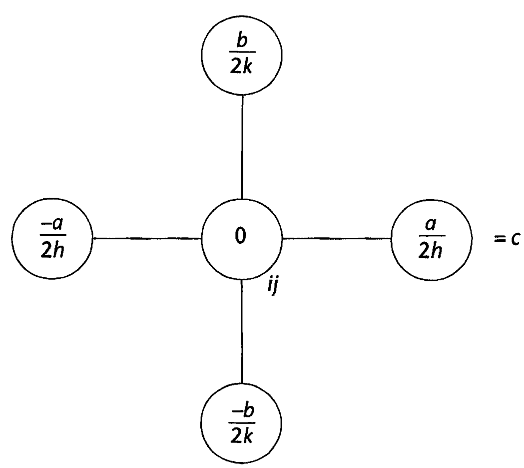
$$\left.\frac{\partial f(x, y)}{\partial x}\right|_{ij} = \frac{f_{i+1,j} - f_{i-1,j}}{2h} \quad \text{and} \quad \left.\frac{\partial f(x, y)}{\partial y}\right|_{ij} = \frac{f_{i,j+1} - f_{i,j-1}}{2k}$$

4 *Computational molecules*

The partial differential equation $a\dfrac{\partial f(x, y)}{\partial x} + b\dfrac{\partial f(x, y)}{\partial y} = c$, evaluated at the ijth grid point, is $a\left.\dfrac{\partial f(x, y)}{\partial x}\right|_{ij} + b\left.\dfrac{\partial f(x, y)}{\partial y}\right|_{ij} = c$ and is by the central difference formula

$$\frac{a}{2h}\left(f_{i+1,j} - f_{i-1,j}\right) + \frac{b}{2k}\left(f_{i,j+1} - f_{i,j-1}\right) = c$$

which is in turn represented by the composite computational molecule:



5 *Numerical solutions*

The solutions are in the form of simultaneous linear equations in that they can be written in matrix form as $\mathbf{Ax} = \mathbf{b}$ with solution $\mathbf{x} = \mathbf{A}^{-1}\mathbf{b}$. Using the *Microsoft Excel* spreadsheet the two functions **MINVERSE(array)** and **MMULT(array1, array2)** are employed.

6 *Derivative boundary conditions*

The grid is extended over the boundary of the function domain by adding additional points outside the domain.

7 *Second-order partial differential equations*

The most general form of a second-order partial differential equation is

$$a(x,y)\frac{\partial^2 f}{\partial x^2} + b(x,y)\frac{\partial^2 f}{\partial x \partial y} + c(x,y)\frac{\partial^2 f}{\partial y^2} + d(x,y)\frac{\partial f}{\partial x} + e(x,y)\frac{\partial f}{\partial y} + g(x,y) = 0$$

Elliptic equations

If $b^2 - 4ac < 0$ then the partial differential equation is called an *elliptic* equation

Hyperbolic equations

If $b^2 - 4ac > 0$ then the partial differential equation is called an *hyperbolic* equation

Parabolic equations

If $b^2 - 4ac = 0$ then the partial differential equation is called a *parabolic* equation.

8 *Second partial derivatives – central difference formulas*

$$\left.\frac{\partial^2 f(x, y)}{\partial x^2}\right|_{ij} \approx \frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{h^2}$$

and $$\left.\frac{\partial^2 f(x, y)}{\partial y^2}\right|_{ij} \approx \frac{f_{i,j-1} - 2f_{i,j} + f_{i,j+1}}{k^2}$$

▶

9 *Time-dependent equations*
To use a central difference formula for the derivative with respect to t would require a knowledge of $f(x, t)$ for values of $t < 0$ and this we do not possess. Consequently, for the derivative with respect to t we use the *forward* difference formula

$$\left.\frac{\partial f(x, t)}{\partial t}\right|_{ij} \approx \frac{f_{i,j+1} - f_{i,j}}{k}$$

So the partial differential equation $\dfrac{\partial^2 f(x, t)}{\partial x^2} = \dfrac{\partial f(x, t)}{\partial t}$ becomes

$$f_{i,j+1} = f_{i,j} + \frac{k}{h^2}(f_{i-1,j} - 2f_{i,j} + f_{i+1,j})$$

where it can be shown that there will be no growth of rounding errors when evaluating this equation if

$$\frac{k}{h^2} \leq \frac{1}{2}.$$

10 *The Crank–Nicolson procedure*
The Crank–Nicolson procedure makes the assumption that the partial differential equation can be satisfied at points in time halfway between two grid points. That is

$$\left.\frac{\partial^2 f(x, t)}{\partial x^2}\right|_{i,j+1/2} = \left.\frac{\partial f(x, t)}{\partial t}\right|_{i,j+1/2}$$

This gives

$$\left.\frac{\partial f(x, t)}{\partial t}\right|_{i,j+1/2} = \frac{f_{i,j+1} - f_{i,j}}{2(k/2)} = \frac{f_{i,j+1} - f_{i,j}}{k}$$

$$\left.\frac{\partial^2 f(x, t)}{\partial x^2}\right|_{i,j+1/2} = \frac{1}{2}\left(\frac{f_{i-1,j} - 2f_{i,j} + f_{i+1,j}}{h^2} + \frac{f_{i-1,j+1} - 2f_{i,j+1} + f_{i+1,j+1}}{h^2}\right)$$

So that

$$-f_{i,j+1} + \frac{k}{2h^2}(f_{i-1,j+1} - 2f_{i,j+1} + f_{i+1,j+1})$$
$$= -f_{i,j} - \frac{k}{2h^2}(f_{i-1,j} - 2f_{i,j} + f_{i+1,j})$$

with no restriction on the value of $\dfrac{k}{2h^2}$.

Can You?

Checklist 13

62

Check this list before and after you try the end of Programme test.

On a scale of 1 to 5 how confident are you that you can: Frames

- Derive the finite difference formulas for the first partial derivatives of a function of two real variables and construct the central finite difference formula to represent a first-order partial differential equation? 1 to 4

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Draw a rectangular grid of points overlaid on the domain of a function of two real variables and evaluate the function at the boundary grid points? 5 to 9

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Construct the computational molecule for a first-order partial differential equation in two real variables and use the molecule to evaluate the solutions to the equation at the grid points interior to the boundary? 10 and 11

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Describe the solution as a set of simultaneous linear equations and use matrices to represent them? 12 and 13

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Invert the coefficient matrix and thereby represent the solution to the partial differential equation as a column matrix? 14 to 19

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Take account of a boundary condition in the form of the derivative normal to the boundary? 20 to 28

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Obtain the central finite difference formulas for the second derivatives of a function of two real variables and construct finite difference formulas for second-order partial differential equations? 29 to 38

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Use the forward difference formula for the first time derivatives in partial differential equations involving time and distance? 39 to 48

  Yes ☐ ☐ ☐ ☐ ☐ *No*

▶

- Use the Crank–Nicolson procedure for a partial differential equation involving a first time derivative? 49 to 59

  Yes ☐ ☐ ☐ ☐ ☐ *No*

- Appreciate the use of dimensional analysis in the conversion of a partial differential equation modelling a physical system into a dimensionless equation? 60

  Yes ☐ ☐ ☐ ☐ ☐ *No*

Test exercise 13

63

1 Solve the following equation numerically.

$$5\frac{\partial f(x, y)}{\partial x} - 4\frac{\partial f(x, y)}{\partial y} = -5$$

for $0 \leq x \leq 1$ with a step length $h = 1/4$ and $0 \leq y \leq 1$ with a step length $k = 1/3$ where

$f(x, 0) = 3x - 4$, $f(x, 1) = 3x + 1$, $f(0, y) = 5y - 4$ and $f(1, y) = 5y - 1$

2 Solve the following equation numerically.

$$10\frac{\partial f(x, y)}{\partial x} + 8\frac{\partial f(x, y)}{\partial y} = -10$$

for $0 \leq x \leq 1$ with a step length $h = 1/3$ and $0 \leq y \leq 1$ with a step length $k = 1/3$ where

$f(x, 0) = 7x + 5$, $f(x, 1) = 7x - 5$, $f(0, y) = 5 - 10y$ and $\left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 7$

3 Name the type of equation in each of the following.

(a) $2\frac{\partial f(x, y)}{\partial x} - 3y\frac{\partial f(x, y)}{\partial y} = 4xy$

(b) $\frac{\partial f(x, y)}{\partial x} + \frac{\partial^2 f(x, y)}{\partial x \partial y} - \frac{\partial f(x, y)}{\partial y} = \frac{x}{y}$

(c) $\frac{\partial^2 f(x, y)}{\partial x^2} - 2\frac{\partial^2 f(x, y)}{\partial x \partial y} + \frac{\partial^2 f(x, y)}{\partial y^2} = 0$

(d) $\frac{\partial}{\partial x}\left[\frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y}\right] = \frac{x^2}{y^3}$

(e) $3\frac{\partial^2 f(x, y)}{\partial x^2} - 2\frac{\partial^2 f(x, y)}{\partial x \partial y} + \frac{\partial^2 f(x, y)}{\partial y^2} = 3xy$

4 Solve the following equation numerically.

$$\frac{\partial^2 f(x, y)}{\partial x^2} + \frac{\partial^2 f(x, y)}{\partial y^2} = -2 \text{ for } 0 \leq x \leq 1 \text{ and } 0 \leq y \leq 1$$

with step lengths $h = k = 1/3$ where

$f(x, 0) = f(x, 1) = x - 2$, $f(0, y) = y^2 - y - 2$ and $\left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 1$

▶

5 Solve the following equation numerically using the forward difference approximation for the first derivative with respect to time.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \le x \le 1$ with a step length $h = 0{\cdot}2$ and $0 \le t \le 0{\cdot}2$ with step length $k = 0{\cdot}02$ where

$$f(x, 0) = x^2,\ f(0, t) = 0 \text{ and } \left.\frac{\partial f(x, t)}{\partial x}\right|_{x=1} = 0{\cdot}25$$

6 Solve the following equation numerically using the Crank–Nicolson procedure.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \le x \le 1$ with a step length $h = 0{\cdot}2$ and $0 \le t \le 0{\cdot}2$ with step length $k = 0{\cdot}04$ where

$$f(x, 0) = x^2 - x + 1 \text{ and } f(0, t) = f(1, t) = 1$$

Further problems 13

64

1 Solve the following equation numerically.

$$-2\frac{\partial f(x, y)}{\partial x} + \frac{\partial f(x, y)}{\partial y} = 0$$

for $0 \le x \le 1$ with a step length $h = 1/4$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$$f(x, 0) = x - 3,\ f(x, 1) = x - 1,\ f(0, y) = 2y - 3 \text{ and } f(1, y) = 2y - 2$$

2 Solve the following equation numerically.

$$9\frac{\partial f(x, y)}{\partial x} - 7\frac{\partial f(x, y)}{\partial y} = -7$$

for $0 \le x \le 1$ with a step length $h = 1/3$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$f(x, 0) = 7x + 4,\ f(x, 1) = 7x + 14,\ f(0, y) = 10y + 4$
and $f(1, y) = 10y + 11$

3 Solve the following equation numerically.

$$x\frac{\partial f(x, y)}{\partial x} + (y + 1)\frac{\partial f(x, y)}{\partial y} = 0$$

for $0 \le x \le 1$ with a step length $h = 1/3$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$f(x, 0) = x - 1,\ f(x, 1) = (x - 2)/2,\ f(0, y) = -1$
and $f(1, y) = -y/(y + 1)$

▶

4 Solve the following equation numerically.

$$\frac{\partial f(x, y)}{\partial y} - \frac{\partial f(x, y)}{\partial x} = x^2 + y^2$$

for $0 \le x \le 1$ with a step length $h = 1/4$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$$f(x, 0) = 0,\ f(x, 1) = x(x-1),\ f(0, y) = 0 \text{ and } f(1, y) = y(1-y)$$

5 Solve the following equation numerically.

$$3\frac{\partial f(x, y)}{\partial x} - 5\frac{\partial f(x, y)}{\partial y} = -4$$

for $0 \le x \le 1$ with a step length $h = 1/3$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$$f(x, 0) = 7x + 15,\ f(x, 1) = 7x + 20,\ f(0, y) = 5y + 15$$

$$\text{and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 7$$

6 Solve the following equation numerically.

$$11\frac{\partial f(x, y)}{\partial x} + 12\frac{\partial f(x, y)}{\partial y} = 19$$

for $0 \le x \le 1$ with a step length $h = 1/3$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$$f(x, 0) = 5x + 21,\ f(x, 1) = 5x + 18,\ f(0, y) = 21 - 3y$$

$$\text{and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 5$$

7 Solve the following equation numerically.

$$2x\frac{\partial f(x, y)}{\partial x} - y\frac{\partial f(x, y)}{\partial y} = 8x^2$$

for $0 \le x \le 1$ with a step length $h = 1/3$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$$f(x, 0) = 2x^2 + 4,\ f(x, 1) = 2x^2 - 3x + 4,\ f(0, y) = 4$$

$$\text{and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 4 - 3y^2$$

8 Solve the following equation numerically.

$$y\frac{\partial f(x, y)}{\partial x} + x\frac{\partial f(x, y)}{\partial y} = x^4 - y^4$$

for $0 \le x \le 1$ with a step length $h = 1/3$ and $0 \le y \le 1$ with a step length $k = 1/3$ where

$$f(x, 0) = 0,\ f(x, 1) = x(x+1)(x-1),\ f(0, y) = 0$$

$$\text{and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = y(3 - y^2)$$

▶

9 Solve the following equation numerically.

$$\frac{\partial^2 f(x, y)}{\partial x^2} + \frac{\partial^2 f(x, y)}{\partial y^2} = -4$$

for $0 \le x \le 1$ and $0 \le y \le 1$ with step lengths $h = k = 1/3$ where

$$f(x, 0) = 3x^2,\ f(x, 1) = 3x^2 - 5,\ f(0, y) = -5y^2 \text{ and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 6$$

10 Solve the following equation numerically.

$$\frac{\partial^2 f(x, y)}{\partial x^2} + \frac{\partial^2 f(x, y)}{\partial y^2} = 2(x + y)$$

for $0 \le x \le 1$ and $0 \le y \le 1$ with step lengths $h = k = 1/3$ where

$$f(x, 0) = -1,\ f(x, 1) = x^2 + 3x - 1,\ f(0, y) = -1$$

and $\left.\dfrac{\partial f(x, y)}{\partial x}\right|_{x=1} = y^2 + 4y$

11 Solve the following equation numerically.

$$\frac{\partial^2 f(x, y)}{\partial x^2} + \frac{\partial^2 f(x, y)}{\partial y^2} = (2 - x^2)\cos y$$

for $0 \le x \le 1$ and $0 \le y \le 1$ with step lengths $h = k = 1/3$ where

$$f(x, 0) = x^2,\ f(x, 1) = 0{\cdot}540302x^2,\ f(0, y) = 0 \text{ and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = 2x\cos y$$

12 Solve the following equation numerically.

$$\frac{\partial^2 f(x, y)}{\partial x^2} - \frac{\partial^2 f(x, y)}{\partial y^2} = 4(x - y)$$

for $0 \le x \le 1$ and $0 \le y \le 1$ with step lengths $h = k = 1/3$ where

$$f(x, 0) = x^3,\ f(x, 1) = (x + 1)(x^2 + 1),\ f(0, y) = y^3$$

and $\left.\dfrac{\partial f(x, y)}{\partial x}\right|_{x=1} = y^2 + 2y + 3$

13 Given the central difference formula

$$\left.\frac{\partial^2 f(x, y)}{\partial x \partial y}\right|_{ij} = \frac{1}{4h^2}(f_{i-1,j-1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i+1,j+1})$$

where the step length in both directions is h, construct the computational molecule for this formula.

Solve the equation

$$\frac{\partial^2 f(x, y)}{\partial x \partial y} = 1$$

for $0 \le x \le 1$ and $0 \le y \le 1$ with step lengths $h = 1/3$ where

$$f(x, 0) = 0,\ f(x, 1) = x,\ f(0, y) = 0 \text{ and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = y$$

▶

14 Given the central difference formula

$$\left.\frac{\partial^2 f(x, y)}{\partial x \partial y}\right|_{ij} = \frac{1}{4h^2}(f_{i-1,j-1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i+1,j+1})$$

where the step length in both directions is h, construct the computational molecule for this formula.

Solve the equation

$$\frac{\partial^2 f(x, y)}{\partial x \partial y} = 2(x - y)$$

for $0 \leq x \leq 1$ and $0 \leq y \leq 1$ with step lengths $h = 1/3$ where

$$f(x, 0) = 0,\ f(x, 1) = x(x-1),\ f(0, y) = 0 \text{ and } \left.\frac{\partial f(x, y)}{\partial x}\right|_{x=1} = y(2 - y)$$

15 Solve the following equation numerically using the forward difference approximation for the first derivative with respect to time.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \leq x \leq 1$ with a step length $h = 0{\cdot}2$ and $0 \leq t \leq 0{\cdot}2$ with a step length $k = 0{\cdot}02$ where

$$f(x, 0) = x(x-1),\ f(0, t) = 2t \text{ and } \left.\frac{\partial f(x, t)}{\partial x}\right|_{x=1} = 1$$

16 Solve the following equation numerically using the forward difference approximation for the first derivative with respect to time.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{1}{0{\cdot}1}\frac{\partial f(x, t)}{\partial t}$$

for $0 \leq x \leq 1$ with a step length $h = 0{\cdot}2$ and $0 \leq t \leq 0{\cdot}2$ with a step length $k = 0{\cdot}02$ where

$$f(x, 0) = \sin x,\ f(0, t) = 0 \text{ and } \left.\frac{\partial f(x, t)}{\partial x}\right|_{x=1} = 0{\cdot}54e^{-t/10}$$

17 Solve the following equation numerically using the forward difference approximation for the first derivative with respect to time.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \leq x \leq 1$ with a step length $h = 0{\cdot}2$ and $0 \leq t \leq 0{\cdot}2$ with a step length $k = 0{\cdot}02$ where

$$f(x, 0) = 3\sin(0{\cdot}64x),\ f(0, t) = 0 \text{ and } \left.\frac{\partial f(x, t)}{\partial x}\right|_{x=1} = 2{\cdot}41e^{-0{\cdot}41t}$$

▶

18 Solve the following equation numerically using the Crank–Nicolson procedure.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \leq x \leq 1$ with a step length $h = 0{\cdot}2$ and $0 \leq t \leq 0{\cdot}6$ with a step length $k = 0{\cdot}04$ where

$$f(x, 0) = x^2 + x - 1 \text{ and } f(0, t) = 2t - 1,\ f(1, t) = 1 + 2t$$

19 Solve the following equation numerically using the Crank–Nicolson procedure.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \leq x \leq 1$ with a step length $h = 0{\cdot}1$ and $0 \leq t \leq 0{\cdot}14$ with a step length $k = 0{\cdot}02$ where

$$f(x, 0) = 10x(x - 1) \text{ and } f(0, t) = f(1, t) = 20t$$

20 Solve the following equation numerically using the Crank–Nicolson procedure.

$$\frac{\partial^2 f(x, t)}{\partial x^2} = \frac{\partial f(x, t)}{\partial t}$$

for $0 \leq x \leq 1$ with a step length $h = 0{\cdot}1$ and $0 \leq t \leq 0{\cdot}6$ with a step length $k = 0{\cdot}04$ where

$$f(x, 0) = 100 \sin \pi x \text{ and } f(0, t) = f(1, t) = 0$$